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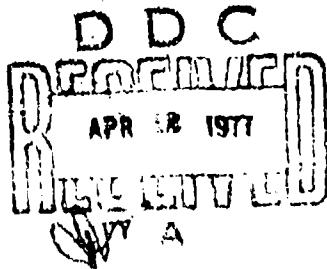
13. Lanthanides in  $\text{YAlO}_3$

February 1977

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Host Lattice Interactions: 13. Lanthanides in  $\text{YAlO}_3$   
Don, Nick Karyotakis, and Donald E. Warren

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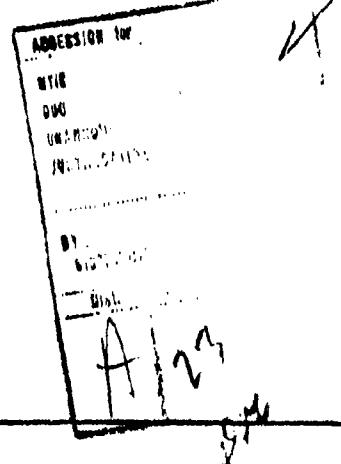
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"The latter  $B_{km}$  are used to calculate the energy levels of the lower J-multiplets for the lanthanide series in  $YAlO_3$ .



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## 1. INTRODUCTION

The optical spectra of a number of triply ionized lanthanides in yttrium orthoaluminate ( $\text{YAlO}_3$ ) have been reported.<sup>1-6</sup> Because of the excellent laser properties of this material,<sup>1</sup> we have examined these reported spectra in order to obtain a unified theory of the crystal field interactions at the laser ion site in  $\text{YAlO}_3$ . In this report, phenomenological crystal field parameters,  $B_{km}$ , for triply ionized Nd, Tb, Dy, Ho, Er, and Tm were obtained by diagonalizing a  $C_s(C_{1h})$  crystal field Hamiltonian in a free-ion wave-function basis. The parameters were reduced to give the part of the crystal field components,  $A_{km}$ , due solely to the crystal lattice, and new  $B_{km}$  were then calculated for all the lanthanides by using previously derived<sup>7</sup>  $\rho_k$ , where  $B_{km} = \rho_k A_{km}$ . These  $B_{km}$  were then used to calculate the energy levels of the lower J-multiplets for the lanthanide series in  $\text{YAlO}_3$ .

## 2. CALCULATIONS

The point group symmetry<sup>8</sup> at the yttrium site in  $\text{YAlO}_3$  is  $C_s(C_{1h})$ , which includes a reflection plane in addition to the identity operation.

<sup>1</sup>M. Bass and M. J. Weber, *Laser Focus*, 7 (1971), 34-36.

<sup>2</sup>M. J. Weber and T. E. Varitimos, *J. Appl. Phys.*, 42 (1971), 4996-5005.

<sup>3</sup>Kh. S. Bagdasarov, A. A. Kaminskii, and G. I. Rogov, *Sov. Phys. Doklady*, 14 (1969), 346-348.

<sup>4</sup>J. L. Berg, *High Resolution Low Temperature Spectra of  $\text{Tb}^{3+}$  in  $\text{YAlO}_3$ , Master's Thesis, Air Force Institute of Technology, Wright-Patterson Air Force Base, OH* (June 1973).

<sup>5</sup>V. A. Antanov, P. A. Arsenev, K. E. Bienert, and A. V. Potemkin, *Phys. Status Solidi A*, 19 (1973), 289-299.

<sup>6</sup>V. L. Donlan and A. A. Santiago, Jr., *J. Chem. Phys.*, 57 (1972), 4717-4723.

<sup>7</sup>D. E. Wortman, C. A. Morrison, and N. Karayianis, *Rare Earth Ion-Host Lattice Interactions II. Lanthanides in  $\text{Y}_3\text{Al}_5\text{O}_12$* , Harry Diamond Laboratories TR-1773 (August 1976).

<sup>8</sup>R. Diehl and G. Brandt, *Materia Research Bulletin*, 10 (1975), 85-90.

If the z-axis is taken perpendicular to the reflection plane, the crystal field Hamiltonian is of the form

$$H_x = \sum_{km} B_{km} C_{km}, \quad k = 2, 4, 6; \quad m = 0, \pm 2, \dots \pm k, \quad (1)$$

where the  $B_{km}$  for  $m \neq 0$  may be complex. With no loss in generality, we chose real  $B_{00}$  and imaginary  $B_{02} \neq 0$ .

The crystal field Hamiltonian was diagonalized in the low-lying J-multiplets of free-ion wave functions,<sup>9</sup> and the  $B_{km}$  were varied to obtain best fits between theoretical and experimental energy levels reported for Nd,<sup>2,3</sup> Tb,<sup>4</sup> Dy,<sup>5</sup> Ho,<sup>5</sup> Er<sup>5,6</sup> and Tm.<sup>5</sup> The resultant best-fit parameters are given in table I, where the next to last four columns give the number of J-multiplets diagonalized, the number of levels in these multiplets, the number of experimental energies used, and finally the rms deviation between these energies and their corresponding theoretical energies. The multiplets included for each ion were (1) the <sup>4</sup>I term, <sup>4</sup>F<sub>3/2</sub>, and <sup>4</sup>F<sub>9/2</sub> for Nd; (2) the <sup>7</sup>F term and <sup>7</sup>D<sub>4</sub> for Tb; (3) <sup>8</sup>H<sub>15/2</sub>, <sup>13/2</sup>, <sup>11/2</sup>, <sup>5/2</sup>, and <sup>6</sup>F<sub>7/2</sub>, <sup>5/2</sup> for Dy; (4) <sup>5</sup>I<sub>8,7,6,5</sub> and <sup>5</sup>F<sub>4,3</sub> for Ho; (5) the <sup>4</sup>I term, <sup>4</sup>F<sub>9/2</sub>, and <sup>4</sup>S<sub>3/2</sub> for Er; and (6) the <sup>3</sup>H term, <sup>3</sup>F<sub>3/2</sub>, and <sup>1</sup>G<sub>4</sub> for Tm. The lack of sufficient data in some cases plus ambiguities owing to overlapping multiplets governed the choice of

<sup>2</sup>M. J. Weber and T. E. Varitimos, *J. Appl. Phys.*, **42** (1971), 4996-5005.

<sup>3</sup>Kh. S. Bagdasarov, A. A. Kaminskii, and G. I. Rogov, *Sov. Phys. Doklady*, **14** (1969), 346-348.

<sup>4</sup>J. L. Berg, *High Resolution Low Temperature Spectra of Tb<sup>3+</sup> in YAlO<sub>3</sub>, Master's Thesis, Air Force Institute of Technology, Wright-Patterson Air Force Base, OH* (June 1973).

<sup>5</sup>V. A. Antanov, P. A. Arsenev, K. E. Bienert, and A. V. Potemkin, *Phys. Status Solidi A*, **19** (1973), 289-299.

<sup>6</sup>V. L. Donlan and A. A. Santiago, Jr., *J. Chem. Phys.*, **57** (1972), 4717-4723.

<sup>9</sup>W. T. Carnall, P. R. Fields, and K. Rajnak, *J. Chem. Phys.*, **49** (1968), 4412-4455.

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TABLE I. PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS,  $B_{km}$ , FOR TRIPLY IONIZED LANTHANIDES IN  $\text{YAlO}_3$

Ion	$E_2$	$B_{2z}$	$B_{2x}$	$B_{3z}$		$B_{3x}$		$B_{3y}$		$B_{4z}$		$B_{4x}$		$B_{4y}$	
				Real	Imagi-										
La <sup>+</sup>	514	-135	-521	525	-214	-515	-111	-348	-155	114	-231	310	-12	310	23
Tb <sup>+</sup>	567	-233	-1063	-217	497	-393	-32	-731	-317	-455	-75	-503	-233	32	55
Dy <sup>+</sup>	553	-163	-382	-616	330	151	-435	-355	156	-233	643	-97	-443	-6	31
Ho <sup>+</sup>	716	-248	-938	-544	384	-63	-363	-263	211	-244	41	553	-751	19	56
Er <sup>+</sup>	547	-3	-793	-467	391	-62	-45	-877	-375	-175	213	53	-255	17	33
Er <sup>+</sup>	431	-170	-833	-346	365	-213	-739	-742	-241	-180	534	17	-224	2	33
Tm <sup>+</sup>	675	-75	-754	-480	567	-42	-5	-751	-772	-154	601	59	-218	-15	32

Notes: 1. The values of  $B_{2z}$  and  $B_{2x}$  are taken from the literature. 2. The values of  $B_{3z}$ ,  $B_{3x}$ , and  $B_{3y}$  are calculated by the method of least squares. 3. The values of  $B_{4z}$ ,  $B_{4x}$ , and  $B_{4y}$  are calculated by the method of least squares.

multiplets and experimental energies that were used in the fitting procedure. Table I, line 6, gives the set of initial  $B_{km}$  for Er that were chosen to begin the fitting procedure. For starting parameters, previously reported parameters for Er:yttrium aluminum garnet (YAG)<sup>10</sup> were used. Since the YAG crystal field is real, imaginary  $B_{kp}$  was arbitrarily set at 200 cm<sup>-1</sup>.

Subsequent choices for starting parameters for the other ions were chosen by scaling the Ho parameters, which were obtained by averaging the best-fit Dy and Er phenomenological  $B_{km}$ , according to the  $\rho_k$  in table II. These  $\rho_k$ , given by

TABLE II. VALUES FOR  $\rho_k = \tau^{-k} \langle r^k \rangle (1 - \sigma_k)$   
IN  $\Delta_k$  TO CONVERT LATTICE SUMS  
CRYSTAL FIELD COMPONENTS,  $A_{km}$ ,  
TO CRYSTAL FIELD PARAMETERS,  $B_{km}$ ,  
AS  $B_{km} = \rho_k A_{km}$

Ion	$\rho_c$	$\rho_h$	$\rho_s$
Er	0.1841	0.7936	2.3617
Pr	0.1706	0.6464	1.8794
Nd	0.1706	0.5776	1.5897
Dy	0.1679	0.5339	1.4218
Sr	0.1668	0.5049	1.3210
Eu	0.1666	0.4836	1.2503
Tb	0.1668	0.4656	1.1873
Tb	0.1673	0.4690	1.1732
Dy	0.1681	0.4361	1.0614
Ho	0.1697	0.4217	1.0119
Er	0.1706	0.4126	0.9826
Eu	0.1722	0.4053	0.9649
Tb	0.1737	0.3938	0.9140

<sup>10</sup>C. A. Morrison, D. E. Wortman, and N. Karayianis, *J. Phys. C: Solid State Phys.*, 9 (1976), L191.

$$\rho_k = \tau^{-k} \langle r^k \rangle (1 - \sigma_k) , \quad (2)$$

are rare-earth-ion dependent and relate the  $B_{km}$  to the lattice sum field  $A_{km}$  by

$$B_{km} = \rho_k A_{km} , \quad (3)$$

where it is assumed that the  $A_{km}$  are host dependent only. The  $\langle r^k \rangle$  are smoothed values of Freeman and Watson,<sup>11</sup> the  $\sigma_k$  are linearly interpolated calculations of Erdos and Kang,<sup>12</sup> and the  $\tau$  are quadratically fit wave-function expansion parameters found in studies of lanthanides in CaWO<sub>4</sub>.<sup>13</sup> The  $B_{km}$  for the lanthanide series obtained by using these  $\tau_k$  values of table II in equation (3) and the  $B_{km}$  for Dy and Er of table I are given in table III.

Energy levels calculated by using the  $B_{km}$  of tables I and III for the lowest-lying six to eight multiplets of the lanthanides in YAlO<sub>3</sub> are given in tables IV to XXI.

To make intensity calculations, some estimates of the odd-fold ( $\text{odd-}k$ )  $A_{km}$  are necessary. These can be obtained by appropriate lattice sums.<sup>14</sup> In this work, we have performed the lattice sums for YAlO<sub>3</sub> using the x-ray data of Diehl and Brandt<sup>8</sup> for oxygen charges  $q_0 = -1$  and  $-2$ ; the results are given in table XXII. The one-fold field,  $A_{1m}$ , was not

<sup>8</sup>R. Diehl and G. Brandt, *Materia Research Bulletin*, 10 (1975), 85-90.

<sup>11</sup>A. J. Freeman and R. E. Watson, *Phys. Rev.*, 127 (1962), 2058-2075.

<sup>12</sup>P. Erdos and J. H. Kang, *Phys. Rev. B*, 6 (1972), 3393-3408.

<sup>13</sup>R. P. Leavitt, C. A. Morrison, and D. M. Wortman, *Rare Earth-Ion-Host Crystal Interactions 3. Three-Parameter Theory of Crystal Fields*, Harry Diamond Laboratories TR-1673 (June 1975).

<sup>14</sup>N. Karayianis and C. A. Morrison, *Rare Earth Ion-Host Lattice Interactions 1. Point Charge Lattice Sum in Scheelite*, Harry Diamond Laboratories TR-1648 (October 1973).

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TABLE III. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , FOR TRIPLY IONIZED LANTHANIDES IN  $\text{YAlO}_3$ <sup>a</sup>

included because of its slow convergence. By appropriate rotations of the coordinate system chosen for the calculation of the  $A_{km}$  of table XXII, different sets of  $A_{km}$  can be generated. Thus by appropriate rotation, the sets of  $A_{km}$  for  $q_0 = -1$  and  $-1.5$  given in table XXIII were calculated. Since the  $A_{km}$  are linear functions of  $q_0$ , a value of  $q_0$  can be chosen by using equation (3) and the  $B_k$  of table II to obtain a best fit of calculated  $B_{km}$  to phenomenological  $B_{km}$ . The results of this calculation give  $q_0 = -1.52$ , and the corresponding  $A_{km}$  are reported elsewhere.<sup>15</sup>

### 3. SUMMARY

Reported energy levels for Nd, Tb, Dy, Ho, Er, and Tm were used to obtain phenomenological  $B_{km}$  that yielded least-rms deviations between these levels and levels calculated by using the Hamiltonian given in equation (1) and unpublished theoretical methods and computer programs. These parameters were then scaled to get even- $k$   $B_{km}$  for the entire lanthanide series in  $YAlO_3$ . It is expected that these  $B_{km}$  will at least serve as starting parameters for the analysis of yet unreported ions in  $YAlO_3$ . No intensities were calculated because the symmetry of the  $Y^{3+}$  site was low and because no reasonable higher symmetry approximation could be made as was done<sup>7</sup> for the lanthanides in YAG.

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<sup>7</sup>D. E. Wortman, C. A. Morrison, and N. Karayianis, Rare Earth Ion-Host Lattice Interactions II. Lanthanides in  $Y_3Al_5O_12$ , Harry Diamond Laboratories TR-1773 (August 1976).

<sup>15</sup>N. Karayianis, D. E. Wortman, and C. A. Morrison, Solid State Comm., 18 (1976).

TABLE IV. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS FOR Pr<sup>3+</sup> IN YAlO<sub>3</sub>

PR II: HALO3. SCALING FROM THE EXPERIMENTAL DATA AVERAGING OF AND FOR HOMED RESULTS									
INITIAL STATE AND CUTOFF (K)	Q = -0.05	Q = -0.10	Q = -0.15	Q = -0.20	Q = -0.25	Q = -0.30	Q = -0.35	Q = -0.40	Q = -0.45
5.000 = R2J	-172.000 = R22	-1317.000 = R22	-737.000 = R42	503.000 = R42	-52.000 = R44	-653.000 = R44	252.000 = R66	-385.000 = R66	-252.000 = R66
-1.000.300 = R6	-1.000.300 = R62	-356.000.CC = R62	1097.000 = R64	-75.000 = R64	-385.000 = R66	-75.000 = R66	-385.000 = R66	-385.000 = R66	-385.000 = R66
3H 5	2554.								
3H 6	4527.0								
SF 2	2161.0								
3F 3	6475.0								
AF 4	6972.0								
LG 4	9923.0								
IG 2	16937.0								
		FREE EIN	PCT	PURE	THEO. ENERGY	EXP. ENERGY			
		-185.5	0.0	30.3	471.4	0.3			
		-46.7	0.0	31.5	471.4	0.3			
		1C.2	C.0	32.5	471.4	0.3			
		7L.4	0.0	33.5	471.4	0.3			
		93.4	0.0	44.5	471.4	0.3			
		97.4	0.0	45.5	471.4	0.3			
		77.4	0.0	46.5	471.4	0.3			
		312.4	0.0	47.5	471.4	0.3			
		457.4	0.0	48.5	471.4	0.3			
		57.4	0.0	49.5	471.4	0.3			
		98.4	0.0	50.5	471.4	0.3			
		10.4	0.0	51.5	471.4	0.3			
		249.4	0.0	52.5	471.4	0.3			
		2161.4	0.0	53.5	471.4	0.3			
		2162.4	0.0	54.5	471.4	0.3			
		2163.4	0.0	55.5	471.4	0.3			
		2164.4	0.0	56.5	471.4	0.3			
		2165.4	0.0	57.5	471.4	0.3			
		2166.4	0.0	58.5	471.4	0.3			
		2167.4	0.0	59.5	471.4	0.3			
		2168.4	0.0	60.5	471.4	0.3			
		2169.4	0.0	61.5	471.4	0.3			
		2170.4	0.0	62.5	471.4	0.3			
		2171.4	0.0	63.5	471.4	0.3			
		2172.4	0.0	64.5	471.4	0.3			
		2173.4	0.0	65.5	471.4	0.3			
		2174.4	0.0	66.5	471.4	0.3			
		2175.4	0.0	67.5	471.4	0.3			
		2176.4	0.0	68.5	471.4	0.3			
		2177.4	0.0	69.5	471.4	0.3			
		2178.4	0.0	70.5	471.4	0.3			
		2179.4	0.0	71.5	471.4	0.3			
		2180.4	0.0	72.5	471.4	0.3			
		2181.4	0.0	73.5	471.4	0.3			
		2182.4	0.0	74.5	471.4	0.3			
		2183.4	0.0	75.5	471.4	0.3			
		2184.4	0.0	76.5	471.4	0.3			
		2185.4	0.0	77.5	471.4	0.3			
		2186.4	0.0	78.5	471.4	0.3			
		2187.4	0.0	79.5	471.4	0.3			
		2188.4	0.0	80.5	471.4	0.3			
		2189.4	0.0	81.5	471.4	0.3			
		2190.4	0.0	82.5	471.4	0.3			
		2191.4	0.0	83.5	471.4	0.3			
		2192.4	0.0	84.5	471.4	0.3			
		2193.4	0.0	85.5	471.4	0.3			
		2194.4	0.0	86.5	471.4	0.3			
		2195.4	0.0	87.5	471.4	0.3			
		2196.4	0.0	88.5	471.4	0.3			
		2197.4	0.0	89.5	471.4	0.3			
		2198.4	0.0	90.5	471.4	0.3			
		2199.4	0.0	91.5	471.4	0.3			
		2200.4	0.0	92.5	471.4	0.3			
		2201.4	0.0	93.5	471.4	0.3			
		2202.4	0.0	94.5	471.4	0.3			
		2203.4	0.0	95.5	471.4	0.3			
		2204.4	0.0	96.5	471.4	0.3			
		2205.4	0.0	97.5	471.4	0.3			
		2206.4	0.0	98.5	471.4	0.3			
		2207.4	0.0	99.5	471.4	0.3			
		2208.4	0.0	100.5	471.4	0.3			
		2209.4	0.0	101.5	471.4	0.3			
		2210.4	0.0	102.5	471.4	0.3			
		2211.4	0.0	103.5	471.4	0.3			
		2212.4	0.0	104.5	471.4	0.3			
		2213.4	0.0	105.5	471.4	0.3			
		2214.4	0.0	106.5	471.4	0.3			
		2215.4	0.0	107.5	471.4	0.3			
		2216.4	0.0	108.5	471.4	0.3			
		2217.4	0.0	109.5	471.4	0.3			
		2218.4	0.0	110.5	471.4	0.3			
		2219.4	0.0	111.5	471.4	0.3			
		2220.4	0.0	112.5	471.4	0.3			
		2221.4	0.0	113.5	471.4	0.3			
		2222.4	0.0	114.5	471.4	0.3			
		2223.4	0.0	115.5	471.4	0.3			
		2224.4	0.0	116.5	471.4	0.3			
		2225.4	0.0	117.5	471.4	0.3			
		2226.4	0.0	118.5	471.4	0.3			
		2227.4	0.0	119.5	471.4	0.3			
		2228.4	0.0	120.5	471.4	0.3			
		2229.4	0.0	121.5	471.4	0.3			
		2230.4	0.0	122.5	471.4	0.3			
		2231.4	0.0	123.5	471.4	0.3			
		2232.4	0.0	124.5	471.4	0.3			
		2233.4	0.0	125.5	471.4	0.3			
		2234.4	0.0	126.5	471.4	0.3			
		2235.4	0.0	127.5	471.4	0.3			
		2236.4	0.0	128.5	471.4	0.3			
		2237.4	0.0	129.5	471.4	0.3			
		2238.4	0.0	130.5	471.4	0.3			
		2239.4	0.0	131.5	471.4	0.3			
		2240.4	0.0	132.5	471.4	0.3			
		2241.4	0.0	133.5	471.4	0.3			
		2242.4	0.0	134.5	471.4	0.3			
		2243.4	0.0	135.5	471.4	0.3			
		2244.4	0.0	136.5	471.4	0.3			
		2245.4	0.0	137.5	471.4	0.3			
		2246.4	0.0	138.5	471.4	0.3			
		2247.4	0.0	139.5	471.4	0.3			
		2248.4	0.0	140.5	471.4	0.3			
		2249.4	0.0	141.5	471.4	0.3			
		2250.4	0.0	142.5	471.4	0.3			
		2251.4	0.0	143.5	471.4	0.3			
		2252.4	0.0	144.5	471.4	0.3			
		2253.4	0.0	145.5	471.4	0.3			
		2254.4	0.0	146.5	471.4	0.3			
		2255.4	0.0	147.5	471.4	0.3			
		2256.4	0.0	148.5	471.4	0.3			
		2257.4	0.0	149.5	471.4	0.3			
		2258.4	0.0	150.5	471.4	0.3			
		2259.4	0.0	151.5	471.4	0.3			
		2260.4	0.0	152.5	471.4	0.3			
		2261.4	0.0	153.5	471.4	0.3			
		2262.4	0.0	154.5	471.4	0.3			
		2263.4	0.0	155.5	471.4	0.3			
		2264.4	0.0	156.5	471.4	0.3			
		2265.4	0.0	157.5	471.4	0.3			
		2266.4	0.0	158.5	471.4	0.3			
		2267.4	0.0	159.5	471.4	0.3			
		2268.4	0.0	160.5	471.4	0.3			
		2269.4	0.0	161.5	471.4	0.3			
		2270.4	0.0	162.5	471.4	0.3			
		2271.4	0.0	163.5	471.4	0.3			
		2272.4	0.0	164.5	471.4	0.3			
		2273.4	0.0	165.5	471.4	0.3			
		2274.4	0.0	166.5	471.4	0.3			
		2275.4	0.0	167.5	471.4	0.3			
		2276.4	0.0	168.5	471.4	0.3			
		2277.4	0.0	169.5	471.4	0.3			
		2278.4	0.0	170.5	471.4	0.3			
		2279.4	0.0	171.5	471.4	0.3			
		2280.4	0.0	172.5	471.4	0.3			
		2281.4	0.0	173.5	471.4	0.3			
		2282.4	0.0	174.5	471.4	0.3			
		2283.4	0.0	175.5	471.4	0.3			
		2284.4	0.0	176.5	471.4	0.3			
		2285.4	0.0	177.5	471.4	0.3			
		2286.4	0.0	178.5	471.4	0.3			
		2287.4	0.0	179.5	471.4	0.3			
		2288.4	0.0	180.5	471.4	0.3			
		2289.4	0.0	181.5	471.4	0.3			
		2290.4	0.0	182.5	471.4	0.3			
		2291.4	0.0	183.5	471.4	0.3			
		2292.4	0.0	184.5	471.4	0.3			
		2293.4	0.0	185.5	471.4	0.3			
		2294.4	0.0	186.5	471.4	0.3			
		2295.4	0.0	187.5	471.4	0.3			
		2296.4	0.0	188.5	471.4	0.3			
		2297.4	0.0	189.5	471.4	0.3			
		2298.4	0.0	190.5	471.4	0.3			
		2299.4	0.0	191.5	471.4	0.3			
		2300.4	0.0	192.5	471.4	0.3			
		2301.4	0.0	193.5	471.4	0.3			
		2302.4	0.0	194.5	471.4	0.3			
		2303.4	0.0	195.5	47				

<sup>a</sup> See footnote at end of table.

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TABLE IV. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS FOR  $Pr^{3+}$  IN  $YAlO_3^a$  (CONT'D)

	FREE ION	PCF	PURE	2M <sub>U</sub>	THEO. ENERGY	EXP. ENERGY
55	16.4		$D_{10}^{-4}$	2	9520.5	0.0
56	17.4		$D_{10}^{-3}$	2	9603.6	0.0
57	17.4		$D_{10}^{-2}$	0	9721.3	0.0
58	17.4		$D_{10}^{-1}$	0	9795.6	0.0
59	17.4		$D_{10}^{-0}$	0	9894.3	0.0
60	17.4		$D_{10}^{-1}$	2	10378.6	0.0
61	17.4		$D_{10}^{-2}$	0	10164.4	0.0
62	17.4		$D_{10}^{-3}$	0	10255.4	0.0
63	17.4		$D_{10}^{-4}$	0	10307.3	0.0
64	18.2		$D_{10}^{-1}$	0	16432.2	0.0
65	19.2		$D_{10}^{-2}$	0	16115.0	0.0
66	19.2		$D_{10}^{-1}$	2	16777.1	0.0
67	19.2		$D_{10}^{-0}$	2	17515.0	0.0
68	19.2		$D_{10}^{-1}$	0	17114.9	0.0

<sup>a</sup> These  $B_{km}$  values were obtained by scaling the  $H_0$  parameters by the  $\gamma_k$  value of table II. The  $H_0$  parameters were obtained by a linear interpolation of the  $D_g$  and  $E_g$  phenomenological  $B_{km}$  values.

TABLE V. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR Nd<sup>3+</sup> IN YAlO<sub>3</sub><sup>d</sup>

ND <sup>3+</sup> YALO <sub>3</sub> DATA 6 MULTIPLETS	3K <sup>a</sup> FROM DV & FR HOM <sup>b</sup>	3/16/75	ND <sup>3+</sup> YALO <sub>3</sub> DATA 6 MULTIPLETS	3K <sup>a</sup> FROM DV & FR HOM <sup>b</sup>	3/16/75
FINAL P <sub>FM</sub> AND C <sub>EFM</sub> , 1.05, 3 = 5.7e-6	3 = .22	-1346.531 = 840	221.130 = 242	325.262 = 642	-214.375 = 344
P <sub>116.325</sub> = .323	-115.335 = .222	1214.435 = 362	221.375 = 864	-82.365 = 866	310.375 = 866
-1.11.346.3 = .663	-34.7.375 = .662	1214.435 = .662			
41 9J/2	336.1				
41 11J/2	221.130				
41 11J/2	221.130				
41 11J/2	41.31.3				
41 11J/2	61.31.3				
4F 3J/2	1146.531				
4F 3J/2	1.750.3				
FREE ENERGIES					
P <sub>EF</sub> P <sub>FM</sub>					
1 4I 7J/2	P <sub>116.3</sub>	1	19 4115/2	3P+4	3746.0*
2 6I 3J/2	P <sub>9.3</sub>	1	20 4115/2	5e-7	5.31.0
3 4I 9J/2	P <sub>6.6</sub>	1	21 4115/2	0.15.2	6011.0
4 4I 9J/2	P <sub>7.6</sub>	1	22 4115/2	0.15.2	6197.0
5 4I 9J/2	P <sub>5.7</sub>	1	23 4115/2	6.46.3	6242.0
6 4I 11J/2	P <sub>7.4</sub>	1	24 4115/2	6.17.0	6311.0*
7 4I 11J/2	P <sub>6.4</sub>	1	25 4115/2	-0.0	-0.0
8 4I 11J/2	P <sub>7.3</sub>	1	26 4115/2	6.92.0	6.92.0
9 4I 11J/2	P <sub>7.3</sub>	1	27 4F 3/2	1141.0	1141.0
10 4I 11J/2	P <sub>5.4</sub>	1	28 4F 3/2	1154.0	1154.0
11 4I 11J/2	P <sub>6.4</sub>	1	29 4F 1/2	3.4.1	3.4.1
12 4I 13J/2	P <sub>7.7</sub>	1	30 4F 1/2	14680.0	14680.0
13 4I 13J/2	P <sub>6.7</sub>	1	31 4F 1/2	14730.0	14730.0
14 4I 13J/2	P <sub>6.5</sub>	1	32 4F 1/2	1475.0	1475.0
15 4I 13J/2	P <sub>6.7</sub>	1	33 4F 1/2	14927.0	14927.0
16 4I 13J/2	P <sub>6.7</sub>	1			
17 4I 13J/2	P <sub>6.8</sub>	1			
18 4I 13J/2	P <sub>6.8</sub>	1			
CENTRIFUGAL ENERGY =					
FREQUENCY =					

<sup>a</sup>The calculated and experimental energy levels rms deviation is 6.786 cm<sup>-1</sup>.

TABLE VI. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS FOR  $\text{Nd}^{3+}$  IN  $\text{YAl}_3\text{O}_3$ <sup>a</sup>

ND IN VALUE		SCALED $B_{km}$ FROM HO DETERMINED BY AVERAGING DV AND ER MODELED RESULTS			
INIT.	$B_{km}$ AND CENTERED	$Q = -0.000$			
546.000	= 82J	-167.000 = 92J	-1178.000 = 84C	-653.000 = 842	-67.000 = 344
-1279.000	= 86J	-66.000 = 862	-101.000 = 864	-63.000 = 866	-326.000 = 866
41 9/2	352.0				
4111/2	2219.0				
4113/2	4192.3				
4115/2	6180.0				
4F 3/2	11500.0				
4F 5/2	12403.0				
2H 9/2 2	12670.0				
4F 7/2	13476.0				
4S 3/2	13583.0				
4F 9/2	14746.3				
		FREE ION	PCT	THEO. ENERGY	EXP. ENERGY
1 41 9/2	97.9	1	2-9	0.0	3457.5
2 41 9/2	34.2	1	167.1	0.0	
3 41 9/2	94.6	1	233.6	0.0	13521.3
4 41 9/2	98.2	1	46C.4	0.0	6.C
5 41 9/2	97.6	1	604.6	0.0	13745.7
6 4111/2	97.4	1	2048.4	0.0	C-C
7 4111/2	96.3	1	2111.4	0.0	4.4664.5
8 4111/2	97.9	1	2158.3	0.0	C-C
9 4111/2	97.3	1	2267.7	0.0	14712.3
10 4111/2	96.4	1	2304.2	0.0	C-C
11 4111/2	97.2	1	2347.4	0.0	14754.3
12 4113/2	97.5	1	3206.7	0.0	14P2R.0
13 4113/2	96.2	1	404C.2	0.0	14P2R.0
14 4113/2	97.0	1	4103.0	0.0	14P2R.0
15 4113/2	97.2	1	4114.2	0.0	14P2R.0
16 4113/2	97.2	1	4253.2	0.0	14P2R.0
17 4113/2	97.1	1	4297.2	0.0	14P2R.0
18 4113/2	98.0	1	4388.2	0.0	14P2R.0
19 4115/2	97.5	1	5778.2	0.0	12314.2
20 4115/2	99.3	1	5873.7	0.0	12314.2
21 4115/2	99.1	1	6012.3	0.0	12314.2
22 4115/2	94.3	1	6131.6	0.0	12314.2
23 4115/2	96.3	1	6276.7	0.0	12314.2
24 4115/2	99.2	1	631P.5	0.0	12314.2
25 4115/2	98.2	1	65G.6	0.0	12314.2
26 4115/2	99.6	1	6595.2	0.0	12314.2

<sup>a</sup> These  $B_{km}$  values were obtained by scaling the Ho parameters by the  $\rho_k$  value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological  $B_{km}$  values.

TABLE VII. CRYSTAL FIELD PARAMETERS,  $B_{\text{eff}}$ , AND ENERGY LEVELS FOR  $\text{Pm}^{3+}$  IN  $\text{YAl}_3$ <sup>a</sup>

<sup>a</sup> See footnote at end of table.

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TABLE VII. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS  
FOR  $\text{Nd}^{3+}$  IN  $\text{YAl}_3$ <sup>a</sup> (CONT'D)

FREE ION	PCT	PURE	2MU	THEO. ENERGY	EXP. ENERGY
57	51	1	3.1	6.721.0	6.721.0
58	51	2	3.4	6.721.7	6.721.7
59	51	3	3.7	6.723.5	6.723.5
60	51	4	4.0	6.724.4	6.724.4
61	51	5	4.3	6.725.3	6.725.3
62	51	6	4.6	6.726.2	6.726.2
63	51	7	4.9	6.727.1	6.727.1
64	51	8	5.2	6.728.0	6.728.0
65	51	9	5.5	6.728.9	6.728.9
66	56	1	3.6	12.644.4	12.644.4
67	56	2	3.9	12.644.1	12.644.1
68	57	1	3.7	12.644.0	12.644.0

<sup>a</sup> These  $B_{km}$  values were obtained by scaling the Ho parameters by the  $\alpha_k$  value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological  $B_{km}$  values.

TABLE VIII. CRYSTAL FIELD PARAMETERS,  $B_{\text{eff}}$ , AND ENERGY LEVELS FOR  $\text{Sm}^{3+}$  IN  $\text{YAlO}_3$ <sup>a</sup>

See Fig. 1. Values, scaled from Fig. 4 by (permitted by averaging over and for fitted results)											
1M11, EPR AND CENTERED.	$Q = 0.00$										
536-300 = 82J	-164-030 = 1.2	-1625-000 = 840	-575-000 = 842	397-000 = 842	-41-000 = 844	-666-000 = 866	-271-000 = 866	-666-000 = 866	-177-000 = 866	-666-000 = 866	-666-000 = 866
-1064-000 = 80J	-52-000 = 80J	-251-000 = 862	773-000 = 864	-52-000 = 864	-271-000 = 864	-666-000 = 866	-177-000 = 866	-666-000 = 866	-177-000 = 866	-666-000 = 866	-666-000 = 866
6H 5/2	134-0										
6H 7/2	114-3-1										
6H 9/2	23-32-1										
6H 11/2	37-37-0										
6H 13/2	50-32-0										
6F 1/2	63-52-0										
6H 15/2	65-50-0										
6H 17/2	67-00-0										
6F 3/2	71-16-0										
6F 7/2	79-35-0										
6F 9/2	91-47-0										
		FREE ENERGY	PCT ENERGY	2NU	THEO. ENERGY	FIT. ENERGY					
1	6H 5/2	97-1	1	-67-4	0-0	19-6-13/2	37-7	1	4-1-92-3	0-0	0-0
2	6H 7/2	96-5	1	94-1	0-0	20-0-13/2	36-2	1	4-1-77-1	0-0	0-0
3	6H 9/2	97-0	1	91-4	0-0	21-6-13/2	32-7	1	5-2-5-7	0-0	0-0
4	6H 11/2	95-4	1	88-5	0-0	22-6-13/2	35-0	1	5-6-1-4	0-0	0-0
5	6H 13/2	95-6	1	81-3	0-0	23-6-13/2	37-4	1	5-1-1-3	0-0	0-0
6	6F 1/2	95-7	1	73-7	0-0	24-6-13/2	37-2	1	2-7-7-5	0-0	0-0
7	6H 15/2	97-0	1	143-7-1	0-0	25-6-13/2	37-3	1	5-3-7-3	0-0	0-0
8	6H 17/2	97-1	1	227-7-1	0-0	26-6-15/2	35-0	1	6-1-15-7	0-0	0-0
9	6H 19/2	96-0	1	231-7-1	0-0	27-6-15/2	35-1	1	6-3-6-2	0-0	0-0
10	6H 21/2	95-1	1	235-7-1	0-0	28-6F 11/2	35-0	1	6-3-6-1	0-0	0-0
11	6F 3/2	97-0	1	245-7-1	0-0						
12	6H 23/2	97-7	1	247-7-1	0-0						
13	6H 11/2	97-0	1	4-8-2-5	0-0						
14	6H 13/2	95-7	1	4-8-2-6	0-0						
15	6H 15/2	97-0	1	4-7-7-6	0-0						
16	6H 17/2	97-1	1	4-7-7-7	0-0						
17	6H 19/2	97-2	1	4-7-7-8	0-0						
18	6H 21/2	97-3	1	4-7-7-9	0-0						

<sup>a</sup> See footnote at end of table.

TABLE VIII. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS FOR  $S_{m}^{+3}$  IN  $YAlO_3$ <sup>a</sup> (CONT'D)

FREE ION	PCT. ERRE	2MU	THEO. ENERGY	EXP. ENERGY
36 6H15/2	6.929	1	6422.3	0.0
37 6F 7/2	3.727	1	7145.8	0.0
38 6F 5/2	3.222	1	7176.6	0.0
39 5F 5/2	2.625	1	7236.4	0.0
40 6F 7/2	3.742	1	7380.2	0.0
41 5F 7/2	3.742	1	8618.4	0.0
42 6F 7/2	37.7	1	9549.9	0.0
43 6F 7/2	36.3	1	8116.6	0.0
44 6F 7/2	39.2	1	9115.8	0.0
45 5F 7/2	33.6	1	9157.4	0.0
46 6F 7/2	34.4	1	9192.1	0.0
47 6F 7/2	34.7	1	9216.5	0.0
48 6F 5/2	34.2	1	9245.4	0.0

<sup>a</sup> These  $B_{km}$  values were obtained by scaling the no parameters by the  $\eta_k$  value of table II. The no parameters were obtained by a linear interpolation of the Dy and Er phenomenological  $B_{km}$  values.

TABLE IX. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS FOR  $\text{Eu}^{3+}$  IN  $\text{YAl}_5\text{O}_8$ <sup>a</sup>

EU IN VALUES INIT. $B_{km}$ AND CENTERIDS:		$G = -0.000$		$-163.000 = B_{22}$		$-385.000 = B_{40}$		$-552.000 = B_{42}$		$361.000 = B_{64}$		$-39.000 = B_{44}$		$-639.000 = B_{46}$		$-257.000 = B_{65}$		$-68.000 = B_{66}$	
TF 0	96.0	-1066.000	= B60	-163.000	= B22	-385.000	= B40	-552.000	= B42	361.000	= B64	-39.000	= B44	-639.000	= B46	-257.000	= B65	-68.000 = B66	
TF 0	96.0	-1066.000	= B60	-163.000	= B22	-385.000	= B40	-552.000	= B42	361.000	= B64	-39.000	= B44	-639.000 = B46	-168.000 = B66	-257.000 = B65	-68.000 = B66		
TF 1	413.0																		
TF 2	1175.0																		
TF 3	1998.0																		
TF 4	3000.0																		
TF 5	6073.0																		
TF 6	5094.0																		
TF 0	50.0	3	17220.0																
TF 1	50.1	3	18360.0																
TF 2	50.2	3	21422.0																
TF 3	50.3	3	24453.0																
FREE ION PURITY THEORETICAL ENERGY EXP. ENERGY																			
1 TF 0	97.8	0	52.7	0-C															
2 TF 1	96.3	2	333.5	0-C															
3 TF 1	95.0	2	423.6	0-C															
4 TF 1	96.0	0	525.5	0-C															
5 TF 2	94.0	0	1003.8	0-C															
6 TF 2	96.7	2	1034.7	0-C															
7 TF 2	92.2	2	1115.6	0-C															
8 TF 2	95.0	0	1159.0	0-C															
9 TF 2	96.8	2	1323.9	0-C															
10 TF 3	96.7	2	1402.7	0-C															
11 TF 3	21.0	0	1415.4	0-C															
12 TF 3	36.2	2	1922.1	0-C															
13 TF 3	31.1	0	1452.3	0-C															
14 TF 3	34.0	0	2012.6	0-C															
15 TF 3	33.1	2	2443.4	0-C															
16 TF 3	34.5	2	2063.6	0-C															
17 TF 4	94.4	0	2734.3	0-C															
18 TF 4	74.9	2	2417.2	0-C															
19 TF 4	93.6	0	2691.0	0-C															
20 TF 4	94.6	0	2414.1	0-C															
21 TF 4	95.2	2	2481.2	0-C															
22 TF 4	94.4	0	3083.6	0-C															
23 TF 4	36.0	0	3117.1	0-C															
24 TF 4	96.6	2	3153.0	0-C															
25 TF 4	95.8	2	3211.0	0-C															

<sup>a</sup> See footnote at end of table.

TABLE IX. CRYSTAL FIELD PARAMETERS,  $B_{KM}$ , AND ENERGY LEVELS FOR  $\text{Eu}^{3+}$  IN  $\gamma\text{Al}_2\text{O}_3$  (CONT'D)

	FREE ION	PCT. PUR.	2MU	THEO. ENERGY	EXP. ENERGY
51	SC 1	3	106.4	2	16932. <sup>a</sup>
52	SD 1	3	106.0	2	16255. <sup>a</sup>
53	SC 1	3	106.0	0	16745. <sup>a</sup>
54	SD 2	3	109.3	2	21391. <sup>a</sup>
55	SC 2	3	106.3	2	21435. <sup>a</sup>
56	SC 2	3	106.3	2	21422. <sup>a</sup>
57	SC 2	3	106.2	2	21436. <sup>a</sup>
58	SD 2	3	107.3	2	21454. <sup>a</sup>
59	SD 1	3	106.2	2	24624. <sup>a</sup>
60	SD 3	3	106.3	3	24625. <sup>a</sup>
61	SD 3	3	107.1	2	24531. <sup>a</sup>
62	SD 3	3	106.2	2	24556. <sup>a</sup>
63	SD 3	3	106.2	2	24654. <sup>a</sup>
64	SD 3	3	107.2	2	24531. <sup>a</sup>
65	SD 3	3	106.2	2	24695. <sup>a</sup>

<sup>a</sup> These  $B_{KM}$  values were obtained by scaling the  $B_0$  parameters by the  $\delta_k$  value of table II. The  $\delta_k$  parameters were obtained by a linear interpolation of the Dy and Er phenomenological  $B_{KM}$  values.

TABLE X. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS FOR  $Gd^{3+}$  IN  $YAlO_3$

a These  $B_{km}$  values were obtained by scaling the  $H_0$  parameters by the  $\phi_k$  value of table II. The parameters were obtained by a linear interpolation of the  $D_H$  and  $E_R$  phenomenological  $B_{km}$  values.

TABLE XI. ENERGY LEVELS AND PHENOMENOLOGICAL  $B_{km}$  FOR  $Tb^{3+}$  IN  $YAlO_3$ <sup>a</sup>

TB I <sup>c</sup> : VALU RUSSIAS DATA P MUE VPIPL CY. FINAL 99W AND CENPIPLS- Q = 7-521	4/12/75	PCPE NR. 5	FREE IDM			FREE PCT			THEO. ENERGY EXP. ENERGY EXP. ENERGY		
			460	-742	-217.466 = 642	576-378 = 567	-323.503 = 366	-51.516 = 566	-51.304 = 566	-51.304 = 566	-51.304 = 566
267.335 = 823	-231.157 = 572	-1066.235 = 840	26	7F 4	93.7	2	315.772	-7.0	-7.0	-7.0	-7.0
-751.000 = 860	-317.468 = 362	-4224.368 = 862	27	7F 4	93.7	2	315.772	34.71-C*	34.71-C*	34.71-C*	34.71-C*
TF 6	303.2	745.375 = 664	28	7F 4	93.7	2	315.772	-7.0	-7.0	-7.0	-7.0
TF 5	2322.8	745.375 = 664	29	7F 4	93.7	2	315.772	34.71-C*	34.71-C*	34.71-C*	34.71-C*
TF 4	3566.1	745.375 = 664	30	7F 4	93.7	2	315.772	35.51-C*	35.51-C*	35.51-C*	35.51-C*
TF 3	4601.4	745.375 = 664	31	7F 4	93.7	2	315.772	36.51-C*	36.51-C*	36.51-C*	36.51-C*
TF 2	5224.7	745.375 = 664	32	7F 4	93.7	2	315.772	36.51-C*	36.51-C*	36.51-C*	36.51-C*
TF 1	5533.5	745.375 = 664	33	7F 4	93.7	2	315.772	36.51-C*	36.51-C*	36.51-C*	36.51-C*
TF 0	5639.4	745.375 = 664	34	7F 4	93.7	2	315.772	36.51-C*	36.51-C*	36.51-C*	36.51-C*
SD 4	3	20629.3	PCT 93.2%	2MU	THEO. ENERGY	31	7F 4	93.7	2	315.772	36.51-C*
FREE ICN	PCT 93.2%	2MU	THEO. ENERGY	32	7F 4	93.7	2	315.772	36.51-C*	36.51-C*	36.51-C*
1 TF 6	31.3	9	-2.4	33	7F 4	95.4	2	315.772	-7.0	-7.0	-7.0
2 TF 6	32.4	6	-1.7	34	7F 4	95.4	2	315.772	-7.0	-7.0	-7.0
3 TF 6	95.7	2	-0.5	35	7F 3	13.5	2	473.6-C*	473.6-C*	473.6-C*	473.6-C*
4 TF 5	93.1	3	-0.5	36	7F 3	13.5	2	473.6-C*	473.6-C*	473.6-C*	473.6-C*
5 TF 6	32.1	2	-0.5	37	7F 3	22.4	3	4764.4-C*	4764.4-C*	4764.4-C*	4764.4-C*
6 TF 6	32.1	2	-0.5	38	7F 3	33.1	3	4921.9	4921.9	4921.9	4921.9
7 TF 6	32.1	3	-0.5	39	7F 3	95.5	2	4667.7	4667.7	4667.7	4667.7
8 TF 6	32.1	2	-0.5	40	7F 3	12.3	2	47.3-C*	47.3-C*	47.3-C*	47.3-C*
9 TF 6	34.1	3	-0.5	41	7F 2	31.1	2	5.67-C*	5.67-C*	5.67-C*	5.67-C*
10 TF 6	33.3	2	-0.5	42	7F 2	7C.7	2	5.67-C*	5.67-C*	5.67-C*	5.67-C*
11 TF 6	33.2	2	-0.5	43	7F 2	42.3	2	5.67-C*	5.67-C*	5.67-C*	5.67-C*
12 TF 6	32.1	3	-0.5	44	7F 2	7C.7	2	5.67-C*	5.67-C*	5.67-C*	5.67-C*
13 TF 6	31.2	2	-0.5	45	7F 2	42.3	2	5.67-C*	5.67-C*	5.67-C*	5.67-C*
14 TF 5	94.3	2	2.14.5	2126.C*	46	7F 3	7.4	2.017.7-C*	2.017.7-C*	2.017.7-C*	2.017.7-C*
15 TF 5	93.2	2	2.14.5	2165.C	45	7F 2	7.4	2.017.7-C*	2.017.7-C*	2.017.7-C*	2.017.7-C*
16 TF 5	37.4	3	2147.1	2187.C	45	7F 2	7.4	2.017.7-C*	2.017.7-C*	2.017.7-C*	2.017.7-C*
17 TF 2	36.3	3	2.22.3	2215.C*	46	7F 1	6.7	54.4-C*	54.4-C*	54.4-C*	54.4-C*
18 TF 5	32.2	3	2.247.1	2245.C	47	7F 1	6.7	54.4-C*	54.4-C*	54.4-C*	54.4-C*
19 TF 2	37.1	2	2.267.1	2264.C	48	7F 1	6.7	54.4-C*	54.4-C*	54.4-C*	54.4-C*
20 TF 5	39.7	2	2.275.2	2273.C	49	7F 1	6.7	54.4-C*	54.4-C*	54.4-C*	54.4-C*
21 TF 5	37.2	2	2.377.0	-7.0	50	7F 1	6.7	54.4-C*	54.4-C*	54.4-C*	54.4-C*
22 TF 5	37.2	2	2.377.0	-7.0	51	7F 1	6.7	54.4-C*	54.4-C*	54.4-C*	54.4-C*
23 TF 5	26.4	2	2.624.0	2624.C	52	7F 4	1.4	2.017.7-C*	2.017.7-C*	2.017.7-C*	2.017.7-C*
24 TF 5	37.6	2	2.715.2	2715.C	53	7F 4	1.4	2.017.7-C*	2.017.7-C*	2.017.7-C*	2.017.7-C*
					54	7F 4	1.4	2.017.7-C*	2.017.7-C*	2.017.7-C*	2.017.7-C*
					55	7F 4	1.4	2.017.7-C*	2.017.7-C*	2.017.7-C*	2.017.7-C*
					56	7F 4	1.4	2.017.7-C*	2.017.7-C*	2.017.7-C*	2.017.7-C*
					57	7F 4	1.4	2.017.7-C*	2.017.7-C*	2.017.7-C*	2.017.7-C*
					58	7F 4	1.4	2.017.7-C*	2.017.7-C*	2.017.7-C*	2.017.7-C*
					59	7F 4	1.4	2.017.7-C*	2.017.7-C*	2.017.7-C*	2.017.7-C*

<sup>a</sup>The least rms deviation between the calculated and experimental energy levels is 7.521 cm<sup>-1</sup>.

TABLE XI. CRYSTAL FIELD PARAMETERS,  $B_{K\alpha}$ , AND ENERGY LEVELS FOR  $Tb^{3+}$  IN  $YAlO_4$

SCALED DATA DETERMINED BY AVERAGING DAY AND NIGHT RESULTS									
TYPE IN VALUES	SCALED DATA FROM EQUATIONS DETERMINED	Q = -C <sub>1</sub> CCU	-215.00G = B40	-512.00G = B42	353.00G = B42	-36.000 = B44	-592.00G = B46	-164.000 = B64	-231.000 = B66
INIT. BEM ANC CENTRIFUGAL	-164.000	0.22	-215.00G	840	353.00G	842	-36.000	844	-592.00G
530.000 R20	-530.000	0.00	-213.00G	862	-44.000	864	-231.000	866	-151.000
-506.000 = New	-47.000	0.00	-215.00G	862	-36.000	864	-231.000	866	-151.000
TF 6	310.3								
TF 5	2347.0								
TF 4	3580.0								
TF 3	4573.0								
TF 2	5155.0								
TF 1	5432.0								
TF 0	5766.0								
SD 4	3 20569.0								
SD 3	26357.0								
FREE IRON PURITY THEO. ENERGY EXP. ENERGY									
1 TF 6	36.2	0.0	25 TF 4	33.75.6	2	33.75.6	2	34.25.5	0.0
2 TF 6	36.3	0.0	26 TF 4	38.0	2	34.65.7	0.0	34.65.7	0.0
3 TF 6	36.9	0.0	27 TF 4	97.4	2	34.65.6	0.0	34.65.6	0.0
4 TF 6	186.9	0.0	28 TF 4	95.2	2	35.1.3	2.0	35.1.3	2.0
5 TF 6	194.0	0.0	29 TF 4	95.7	2	35.1.3	2.0	35.1.3	2.0
6 TF 6	98.7	0.0	30 TF 4	95.0	0	36.47.1	0.0	36.47.1	0.0
7 TF 6	214.7	0.0	31 TF 4	94.4	1	36.69.4	0.0	36.69.4	0.0
8 TF 6	93.4	0.0	32 TF 4	96.1	2	37.71.2	0.0	37.71.2	0.0
9 TF 6	253.5	0.0	33 TF 4	96.3	0	34.10.4	0.0	34.10.4	0.0
10 TF 6	93.3	0.0	34 TF 4	95.3	0	34.10.4	0.0	34.10.4	0.0
11 TF 6	310.1	0.0	35 TF 4	95.3	0	34.10.4	0.0	34.10.4	0.0
12 TF 6	98.7	0.0	36 TF 4	95.3	0	34.10.4	0.0	34.10.4	0.0
13 TF 6	33.3	0.0	37 TF 4	95.3	0	34.10.4	0.0	34.10.4	0.0
6 TF 6	343.7	0.0	38 TF 4	95.3	0	34.10.4	0.0	34.10.4	0.0
9 TF 5	48.3	0.0	39 TF 4	95.3	0	34.10.4	0.0	34.10.4	0.0
10 TF 6	99.1	0	40 TF 4	95.3	0	34.10.4	0.0	34.10.4	0.0
11 TF 6	99.6	2	41 TF 2	96.3	3	50.04.0	0.0	50.04.0	0.0
12 TF 6	39.1	0	42 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0
13 TF 6	99.7	2	43 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0
14 TF 5	32.0	2	44 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0
15 TF 5	2205.6	2	45 TF 2	97.0	2	50.04.0	0.0	50.04.0	0.0
16 TF 5	36.0	2	46 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0
17 TF 5	36.0	0	47 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0
18 TF 5	36.0	0	48 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0
19 TF 5	97.3	2	49 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0
20 TF 5	312.5	0	50 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0
21 TF 5	37.1	0	51 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0
22 TF 5	95.3	2	52 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0
23 TF 5	97.3	2	53 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0
24 TF 5	98.7	0	54 TF 2	97.0	2	51.71.2	0.0	51.71.2	0.0

<sup>a</sup> See footnote at end of table.

TABLE XII. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS FOR  $Tb^{3+}$  IN  $YAlO_3$ <sup>a</sup> (CONT'D)

FREE ION	PCI	PURE	2HU	THEO. ENERGY	EXP. ENERGY
46 FF 1		94.3	0	2497.1	0.C
47 FF 1		92.9	2	54491.3	0.C
48 FF 1		96.5	2	55773.3	0.C
49 FF 0		95.0	0	54220.4	0.C
50 50 4	3	102.0	2	20512.7	0.C
51 50 4	3	100.7	0	20222.6	0.C
52 50 5	3	108.0	2	20574.3	0.C
53 50 4	3	109.5	0	20534.4	0.C
54 50 4	3	108.0	0	20553.0	0.C
55 50 4	3	102.0	2	20592.1	0.C
56 50 4	3	100.0	0	20616.7	0.C
57 50 4	3	108.0	0	20626.9	0.C
58 50 4	3	103.0	2	20628.6	0.C
59 50 3	3	100.5	0	26334.1	0.C
60 50 3	3	103.0	2	26347.1	0.C
61 50 3	3	100.0	2	26354.6	0.C
62 50 3	3	100.0	0	26357.1	0.C
63 50 3	3	100.0	0	26365.4	0.C
64 50 3	3	100.0	2	26365.1	0.C
65 50 3	3	100.0	0	26373.7	0.C

<sup>a</sup> These  $B_{km}$  values were obtained by scaling the Ho parameters by the  $\rho_K$  value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological  $B_{km}$  values.

TABLE XIII. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR  $Dy^{3+}$  IN  $YAlO_3$ <sup>a</sup>

2Y 1 <sup>+</sup> YAl <sup>+</sup> RUSSIAN DATA MULTIPLET 9/15/75											
FINAL	2K <sup>+</sup> AND CFMPCLES.	2	2.01,	2	2.22	2	2.42	2	2.64	2	2.86
2Y 2 <sup>+</sup> 5G <sub>6</sub> = 4.20	-162.998	= .722	-8E-424 = 84C	-615.005 = 242	239.183 = 842	-151.344 = 344	-440.255 = 864	-4C4-1C7 = 344	48.157 = 966		
-3.94.394 = 561	156.G11 = .767		-7C4-3C11 = .762	647.533C = .764	-96.759 = .664						
6M15/2	2e4-3										
6M13/2	3721.1										
5F11/2	6576.1										
6F 7/2	10392.0										
6F 5/2	11166.1										
5F 3/2	124.16.4										
FREE ION		PCT	PURE	ZNU	THEO. ENERGY	EXP. ENERGY					
1	15/2	1		2.1	1.1	1.1	1.1	1.1	1.1	1.1	1.1
2	6F 15/2	.767	1	5.1	4.0	4.0	4.0	4.0	4.0	4.0	4.0
3	6F 13/2	.761	1	13.6	14.2	14.2	14.2	14.2	14.2	14.2	14.2
4	6F 11/2	.764	1	2.7	2.7	2.7	2.7	2.7	2.7	2.7	2.7
5	6F 9/2	.763	1	22.6	22.6	22.6	22.6	22.6	22.6	22.6	22.6
6	6F 7/2	.765	1	23.8	23.8	23.8	23.8	23.8	23.8	23.8	23.8
7	6F 5/2	.766	1	3.2	3.2	3.2	3.2	3.2	3.2	3.2	3.2
8	6F 3/2	.767	1	4.8	4.8	4.8	4.8	4.8	4.8	4.8	4.8
9	6F 1/2	.768	1	6.1	6.1	6.1	6.1	6.1	6.1	6.1	6.1
10	6I 13/2	.769	1	35.4	35.4	35.4	35.4	35.4	35.4	35.4	35.4
11	6I 11/2	.770	1	35.7	35.7	35.7	35.7	35.7	35.7	35.7	35.7
12	6I 9/2	.771	1	36.6	36.6	36.6	36.6	36.6	36.6	36.6	36.6
13	6I 7/2	.772	1	37.4	37.4	37.4	37.4	37.4	37.4	37.4	37.4
14	6I 5/2	.773	1	37.6	37.6	37.6	37.6	37.6	37.6	37.6	37.6
15	6I 3/2	.774	1	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7
16	6I 1/2	.775	1	5.1	5.1	5.1	5.1	5.1	5.1	5.1	5.1
17	6P 11/2	.776	1	5.4	5.4	5.4	5.4	5.4	5.4	5.4	5.4
18	6P 9/2	.777	1	5.4	5.4	5.4	5.4	5.4	5.4	5.4	5.4
19	6P 7/2	.778	1	5.7	5.7	5.7	5.7	5.7	5.7	5.7	5.7
20	6P 5/2	.779	1	5.8	5.8	5.8	5.8	5.8	5.8	5.8	5.8
21	6P 3/2	.780	1	6.1	6.1	6.1	6.1	6.1	6.1	6.1	6.1
22	6P 1/2	.781	1	6.4	6.4	6.4	6.4	6.4	6.4	6.4	6.4
23	6F 5/2	.782	1	10.337	10.337	10.337	10.337	10.337	10.337	10.337	10.337
24	6F 3/2	.783	1	10.371	10.371	10.371	10.371	10.371	10.371	10.371	10.371

<sup>a</sup>The least-rms deviation between the calculated and experimental energy levels is 8.010  $\text{cm}^{-1}$ .

TABLE XIV. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS FOR  $Dy^{3+}$  IN  $YAlO_3$

<sup>a</sup> These  $B_{km}$  values were obtained by scaling the  $Ro$  parameters by the  $p_k$  value of table II. The  $Ro$  parameters were obtained by a linear interpolation of the Dy and Er phenomenological  $B_{km}$  values.

TABLE XV. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR  $\text{Ho}^{3+}$  IN  $\text{YAlO}_3$

HC IN VALUE RUSSIAN DATA		NAME & ID	
$\text{C}_1\text{H}_2\text{O}$ AND CEFICPC155.		9716875	
716.337	x d20	-246.1348 = 822	-A37.569 = 840
-963.432	= 950	2114.39 = 962	-543.630 = 342
31 R	295.1		-40.725 = 864
51 T	5261.3		
21 S	d735.3		
41 S	112-3.7		
FREE EN		REF IDN	
PC1		PCT	
1.51	6	-2.1	6.0
2.51	4	3.2	-0.0
3.51	6	4.1	4.6
4.51	8	5.1	6.1
6.51	2	6.1	6.5
7.51	4	7.1	6.0
8.51	6	8.1	5.5
9.51	8	9.1	5.1
10.51	H	10.1	4.6
11.51	8	11.1	3.9
12.51	6	12.1	3.2
13.51	4	13.1	2.5
14.51	2	14.1	1.8
15.51	0	15.1	1.1
16.51	6	16.1	0.4
17.51	R	17.1	-0.3
PME		2PMU	
THFO		ENF-G	
EXP		ENERGY	
33.51	0	33.7	33.7
34.51	0	34.5	34.5
35.51	6	35.5	35.5
36.51	0	36.5	36.5
37.51	0	37.5	37.5
38.51	4	38.5	38.5
39.51	6	39.5	39.5
40.51	4	40.5	40.5
41.51	6	41.5	41.5
42.51	6	42.5	42.5
43.51	6	43.5	43.5
44.51	6	44.5	44.5
45.51	6	45.5	45.5
46.51	2	46.5	46.5
47.51	5	47.5	47.5
48.51	5	48.5	48.5
49.51	5	49.5	49.5
50.51	5	50.5	50.5
51.51	5	51.5	51.5
52.51	5	52.5	52.5
53.51	5	53.5	53.5
54.51	5	54.5	54.5
55.51	5	55.5	55.5
56.51	5	56.5	56.5
57.51	0	57.5	57.5
58.51	0	58.5	58.5
59.51	0	59.5	59.5
60.51	0	60.5	60.5
61.51	0	61.5	61.5
62.51	0	62.5	62.5
63.51	0	63.5	63.5
64.51	0	64.5	64.5
65.51	0	65.5	65.5
66.51	0	66.5	66.5
67.51	0	67.5	67.5
68.51	0	68.5	68.5
69.51	0	69.5	69.5
70.51	0	70.5	70.5
71.51	0	71.5	71.5
72.51	0	72.5	72.5
73.51	0	73.5	73.5
74.51	0	74.5	74.5
75.51	0	75.5	75.5
76.51	0	76.5	76.5
77.51	0	77.5	77.5
78.51	0	78.5	78.5
79.51	0	79.5	79.5
80.51	0	80.5	80.5
81.51	0	81.5	81.5
82.51	0	82.5	82.5
83.51	0	83.5	83.5
84.51	0	84.5	84.5
85.51	0	85.5	85.5
86.51	0	86.5	86.5
87.51	0	87.5	87.5
88.51	0	88.5	88.5
89.51	0	89.5	89.5
90.51	0	90.5	90.5
91.51	0	91.5	91.5
92.51	0	92.5	92.5
93.51	0	93.5	93.5
94.51	0	94.5	94.5
95.51	0	95.5	95.5
96.51	0	96.5	96.5
97.51	0	97.5	97.5
98.51	0	98.5	98.5
99.51	0	99.5	99.5
100.51	0	100.5	100.5
101.51	0	101.5	101.5
102.51	0	102.5	102.5
103.51	0	103.5	103.5
104.51	0	104.5	104.5
105.51	0	105.5	105.5
106.51	0	106.5	106.5
107.51	0	107.5	107.5
108.51	0	108.5	108.5
109.51	0	109.5	109.5
110.51	0	110.5	110.5
111.51	0	111.5	111.5
112.51	0	112.5	112.5
113.51	0	113.5	113.5
114.51	0	114.5	114.5
115.51	0	115.5	115.5
116.51	0	116.5	116.5
117.51	R	117.5	117.5
118.51	0	118.5	118.5
119.51	0	119.5	119.5
120.51	0	120.5	120.5
121.51	0	121.5	121.5
122.51	0	122.5	122.5
123.51	0	123.5	123.5
124.51	0	124.5	124.5
125.51	0	125.5	125.5
126.51	0	126.5	126.5
127.51	0	127.5	127.5
128.51	0	128.5	128.5
129.51	0	129.5	129.5
130.51	0	130.5	130.5
131.51	0	131.5	131.5
132.51	0	132.5	132.5
133.51	0	133.5	133.5
134.51	0	134.5	134.5
135.51	0	135.5	135.5
136.51	0	136.5	136.5
137.51	0	137.5	137.5
138.51	0	138.5	138.5
139.51	0	139.5	139.5
140.51	0	140.5	140.5
141.51	0	141.5	141.5
142.51	0	142.5	142.5
143.51	0	143.5	143.5
144.51	0	144.5	144.5
145.51	0	145.5	145.5
146.51	0	146.5	146.5
147.51	0	147.5	147.5
148.51	0	148.5	148.5
149.51	0	149.5	149.5
150.51	0	150.5	150.5
151.51	0	151.5	151.5
152.51	0	152.5	152.5
153.51	0	153.5	153.5
154.51	0	154.5	154.5
155.51	0	155.5	155.5
156.51	0	156.5	156.5
157.51	0	157.5	157.5
158.51	0	158.5	158.5
159.51	0	159.5	159.5
160.51	0	160.5	160.5
161.51	0	161.5	161.5
162.51	0	162.5	162.5
163.51	0	163.5	163.5
164.51	0	164.5	164.5
165.51	0	165.5	165.5
166.51	0	166.5	166.5
167.51	0	167.5	167.5
168.51	0	168.5	168.5
169.51	0	169.5	169.5
170.51	0	170.5	170.5
171.51	0	171.5	171.5
172.51	0	172.5	172.5
173.51	0	173.5	173.5
174.51	0	174.5	174.5
175.51	0	175.5	175.5
176.51	0	176.5	176.5
177.51	0	177.5	177.5
178.51	0	178.5	178.5
179.51	0	179.5	179.5
180.51	0	180.5	180.5
181.51	0	181.5	181.5
182.51	0	182.5	182.5
183.51	0	183.5	183.5
184.51	0	184.5	184.5
185.51	0	185.5	185.5
186.51	0	186.5	186.5
187.51	0	187.5	187.5
188.51	0	188.5	188.5
189.51	0	189.5	189.5
190.51	0	190.5	190.5
191.51	0	191.5	191.5
192.51	0	192.5	192.5
193.51	0	193.5	193.5
194.51	0	194.5	194.5
195.51	0	195.5	195.5
196.51	0	196.5	196.5
197.51	0	197.5	197.5
198.51	0	198.5	198.5
199.51	0	199.5	199.5
200.51	0	200.5	200.5
201.51	0	201.5	201.5
202.51	0	202.5	202.5
203.51	0	203.5	203.5
204.51	0	204.5	204.5
205.51	0	205.5	205.5
206.51	0	206.5	206.5
207.51	0	207.5	207.5
208.51	0	208.5	208.5
209.51	0	209.5	209.5
210.51	0	210.5	210.5
211.51	0	211.5	211.5
212.51	0	212.5	212.5
213.51	0	213.5	213.5
214.51	0	214.5	214.5
215.51	0	215.5	215.5
216.51	0	216.5	216.5
217.51	0	217.5	217.5
218.51	0	218.5	218.5
219.51	0	219.5	219.5
220.51	0	220.5	220.5
221.51	0	221.5	221.5
222.51	0	222.5	222.5
223.51	0	223.5	223.5
224.51	0	224.5	224.5
225.51	0	225.5	225.5
226.51	0	226.5	226.5
227.51	0	227.5	227.5
228.51	0	228.5	228.5
229.51	0	229.5	229.5
230.51	0	230.5	230.5
231.51	0	231.5	231.5
232.51	0	232.5	232.5
233.51	0	233.5	233.5
234.51	0	234.5	234.5
235.51	0	235.5	235.5
236.51	0	236.5	236.5
237.51	0	237.5	237.5
238.51	0	238.5	238.5
239.51	0	239.5	239.5
240.51	0	240.5	240.5
241.51	0	241.5	241.5
242.51	0	242.5	242.5
243.51	0	243.5	243.5
244.51	0	244.5	244.5
245.51	0	245.5	245.5
246.51	0	246.5	246.5
247.51	0	247.5	247.5
248.51	0	248.5	248.5
249.51	0	249.5	249.5
250.51	0	250.5	250.5
251.51	0	251.5	251.5
252.51	0	252.5	252.5
253.51	0	253.5	253.5
254.51	0	254.5	254.5
255.51	0	255.5	255.5
256.51	0	256.5	256.5
257.51	0	257.5	257.5
258.51	0	258.5	258.5
259.51	0	259.5	259.5
260.51	0	260.5	260.5
261.51	0	261.5	261.5
262.51	0	262.5	262.5
263.51	0	263.5	263.5
264.51	0	264.5	264.5
265.51	0	265.5	265.5
266.51	0	266.5	266.5
267.51	0	267.5	267.5
268.51	0	268.5	268.5
269.51	0	269.5	269.5
270.51	0	270.5	270.5
271.51	0	271.5	271.5
272.51	0	272.5	272.5
273.51	0	273.5	273.5
274.51	0	274.5	274.5
275.51	0	275.5	275.5
276.51	0	276.5	276.5
277.51	0	277.5	277.5
278.51	0	278.5	278.5
279.51	0	279.5	279.5
280.51	0	280.5	280.5
281.51	0	281.5	281.5
282.51	0	282.5	282.5
283.51	0	283.5	283.5
284.51	0	284.5	284.5
285.51	0	285.5	285.5
286.51	0	286.5	286.5
287.51	0	287.5	287.5
288.51	0	288.5	288.5
289.51	0	289.5	289.5
290.51	0	290.5	290.5
291.51	0	291.5	291.5
292.51	0	292.5	292.5
293.51	0	293.5	293.5
294.51	0	294.5	294.5
295.51	0	295.5	295.5
296.51	0	296.5	296.5
297.51	0	297.5	297.5
298.51	0	298.5	298.5
299.51	0	299.5	299.5
300.51	0	300.5	300.5
301.51	0	301.5	301.5
302.51	0	302.5	302.5
303.51	0		

<sup>a</sup>The least-rms deviation between the calculated and experimental energy levels is 7.033 cm<sup>-1</sup>.

TABLE XVI. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS FOR  $\text{Ho}^{3+}$  IN  $\text{YAlO}_3$ <sup>a</sup>

HO. IN INIT. BKM AND CENTRIDS.	HO. IN VALUES, SCALED FROM HO. REFERRED TO 0 = 0.00J	HO. IN VALUES, SCALED FROM HO. REFERRED TO 0 = 0.00J						HO. IN VALUES, SCALED FROM HO. REFERRED TO 0 = 0.00J					
		166.000 = 82.3	-166.000 = 82.2	-46C.000 = 84.0	-481.000 = 84.2	332.000 = 84.2	-40.00n = 36.4	557.000 = 84.4	-34.000 = 34.4	136.000 = 84.6	-208.000 = 36.6	592.000 = 84.6	-40.00n = 36.4
51 8	169.6	-42.000 = 86.3	-42.000 = 86.2	-192.000 = 86.2	-192.000 = 86.2	-40.00n = 36.4	-40.00n = 36.4	-557.000 = 84.4	-34.000 = 34.4	-136.000 = 84.6	-208.000 = 36.6	592.000 = 84.6	-40.00n = 36.4
51 7	5219.5												
51 6	8717.6												
51 5	11274.7												
51 4	133333.4												
FREE ION PURITY													
THEO. ENERGY EXP.-ENERGY													
1 51 7	99.3	2	-32.1	0.0	33 51 6	99.6	0	99.3	0	99.6	0	99.3	0
2 51 6	99.3	2	-64.4	0.0	34 51 6	99.6	0	99.3	0	99.6	0	99.3	0
3 51 8	100.0	0	-43.5	0.0	35 51 6	99.7	2	99.7	2	99.7	2	99.7	2
4 51 6	99.9	1	-27.1	0.0	36 51 6	99.7	2	99.7	2	99.7	2	99.7	2
5 51 8	99.7	2	51.3	0.0	37 51 6	99.6	0	99.6	0	99.6	0	99.6	0
6 51 6	100.0	0	72.3	0.0	38 51 6	99.6	0	99.6	0	99.6	0	99.6	0
7 51 8	99.8	2	147.3	0.0	39 51 6	99.6	0	99.6	0	99.6	0	99.6	0
8 51 6	100.0	0	177.4	0.0	40 51 6	99.6	0	99.6	0	99.6	0	99.6	0
9 51 8	99.9	2	180.6	0.0	41 51 6	99.6	0	99.6	0	99.6	0	99.6	0
10 51 6	100.0	0	212.1	0.0	42 51 6	99.6	0	99.6	0	99.6	0	99.6	0
11 51 8	100.0	0	216.5	0.0	43 51 6	99.6	0	99.6	0	99.6	0	99.6	0
12 51 9	100.0	0	239.2	0.0	44 51 6	99.6	0	99.6	0	99.6	0	99.6	0
13 51 9	99.9	0	307.2	0.0	45 51 6	99.6	0	99.6	0	99.6	0	99.6	0
14 51 6	99.7	2	322.0	0.0	46 51 5	98.9	2	98.9	2	98.9	2	98.9	2
15 51 8	99.3	0	251.5	0.0	47 51 5	99.1	2	99.1	2	99.1	2	99.1	2
16 51 6	99.9	2	374.4	0.0	48 51 5	99.4	0	99.4	0	99.4	0	99.4	0
17 51 6	99.9	0	386.4	0.0	49 51 5	99.5	0	99.5	0	99.5	0	99.5	0
18 51 7	99.4	0	512.0	0.0	50 51 5	99.6	0	99.6	0	99.6	0	99.6	0
19 51 7	99.5	0	512.1	0.0	51 51 5	99.1	2	99.1	2	99.1	2	99.1	2
20 51 7	99.7	2	513.0	0.0	52 51 5	99.4	0	99.4	0	99.4	0	99.4	0
21 51 7	99.7	2	514.5	0.0	53 51 5	99.0	0	99.0	0	99.0	0	99.0	0
22 51 7	99.7	0	520.1	0.0	54 51 5	99.2	0	99.2	0	99.2	0	99.2	0
23 51 7	99.4	2	521.1	0.0	55 51 5	99.7	2	99.7	2	99.7	2	99.7	2
24 51 7	99.7	0	521.1	0.0	56 51 5	99.2	0	99.2	0	99.2	0	99.2	0
25 51 7	99.7	2	522.0	0.0	57 51 4	99.4	2	99.4	2	99.4	2	99.4	2
26 51 7	99.4	2	523.1	0.0	58 51 4	99.0	0	99.0	0	99.0	0	99.0	0
27 51 7	99.3	0	523.5	0.0	59 51 4	99.7	2	99.7	2	99.7	2	99.7	2
28 51 7	99.3	2	524.4	0.0	60 51 4	99.4	0	99.4	0	99.4	0	99.4	0
29 51 7	99.7	2	528.2	0.0	61 51 4	99.2	0	99.2	0	99.2	0	99.2	0
30 51 7	99.6	0	529.1	0.0	62 51 4	99.3	2	99.3	2	99.3	2	99.3	2
31 51 7	99.3	0	530.1	0.0	63 51 4	99.4	0	99.4	0	99.4	0	99.4	0
32 51 7	99.3	2	540.4	0.0	64 51 4	99.1	2	99.1	2	99.1	2	99.1	2
					65 51 4	99.7	0	99.7	0	99.7	0	99.7	0

<sup>a</sup> These  $B_{km}$  values were obtained by scaling the Ho parameters by the  $p_k$  value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological  $B_{km}$  values.

TABLE XVII. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR  $\text{Er}^{3+}$  IN  $\text{YAlO}_3$ <sup>a</sup>

FERT IN VALO ANDREW'S DATA - HGF		9/10/1944			
FINAL HK AND CFM 14,15,16,17		Q = 15.34*			
546.608 = B2	-7.553 = B22	-742.799 = B40	-487.332 = B42	391.316 = B44	-481.381 = B44
-876.850 = P63	-304.470 = P62	-175.200 = B62	325.166 = B64	203.311 = B66	304.178 = B66
4115/2	264/3				
4115/2	6137/3				
4111/2	10348.4				
41 9/2	12564.3				
41 9/2	15368.5				
45 3/2	16467.2				
12H11/2 2	19192.1				
4F 7/2	20581.5				
5F 2	22229.8				
4F 3/2	22564.5				
FREE ION PET PURGE		THEO. ENERGY EXP. ENERGY			
99.3	-1C-2	0-C	27 4F	9/2	99.3
100.0	57.8	50-C	28 4F	9/2	99-H
100-C	168.8	170-C	29 4F	9/2	99-C
100-C	212.4	217-C	30 4F	9/2	99-H
100-C	275.0	267-C	31 4F	9/2	99-C
100-C	376.0	3P9-C	32 4S	3/2	99-H
100-C	453.9	446-C	33 4S	3/2	96-P
100-C	528.5	525-C	33 4S	3/2	16413.2
100-C			97.2	1	1P486.2
99.0	4115/2	6608-C*	34 2H11/2	2	19116.5
99.0	4115/2	6646-C	35 2H11/2	2	19136.0
99.0	4113/2	6647-C*	36 2H11/2	2	19175.6
99.7	4113/2	669C-C	37 2H11/2	2	19211.7
99.7	4113/2	672C-C	38 2H11/2	2	19265.2
99.7	4113/2	6773-C	39 2H11/2	2	19281.7
99.9	4113/2	6820-C	40 4F	7/2	20555.3
99.8	4113/2	6835-C	41 4F	7/2	20563.0
99.8	4113/2	6P73-C	42 4F	7/2	20591.2
99.7	4111/2	10277-6	10302-C	7	20621.0*
99.7	4111/2	1030C.8	10340-C	7	20694.3
99.7	4111/2	10336.4	10340-C	7	
99.7	4111/2	10354.5	10355-C	7	
99.7	4111/2	10390-C	10410-C	7	
99.6	4111/2	10413.4	10413.4	7	
99.6	4111/2	12374.3	12393-C	7	
99.7	41 9/2	12374.3	12440-C*	47 4F	3/2
99.7	41 9/2	12459.1	12617-C	49 4F	3/2
99.9	41 9/2	12606.6	12642-C	94.7	9/2
99.9	41 9/2	12633-R	12732.5	94.7	9/2
99.8	41 9/2	12642-C	12732.5	94.7	9/2

<sup>a</sup>The least-rms deviation between these calculated and experimental energy levels is 15.385 cm<sup>-1</sup> (48 levels).

TABLE XVIII. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR  $\text{Er}^{3+}$  IN  $\text{YAlO}_3$

EASTERN RUSSIAN PART. MULTIPLET'S. #13775									
FINAL	CAP AND C-13.	INT.	C =	T = 4.5°					
430.400	= 82°.	1.70.	-170.465	= 84°.	-365.812	= 842	365.198	= 844	-7C9-079 = 844
-742.421	= 96.3	-240.367	= 62	-17-C-513	= 362	534.343	= 864	23.210	= 866
4115.7	262.4								223.613 = R66
4115.7	6735.7								
41111.7	10345.5								
41.7	12566.1								
48.7	13364.4								
45.7	14433.8								
FABR. INT.									
1	4157.2	352.9	-5	0.0	22.41	372	372	12492.5	12371.5
1	4157.2	105.4	1	47.7	50.0	73.51	372	372	12444.3
3	4157.2	105.4	1	174.3	170.0	24.41	372	372	12457.4
4	4157.2	105.4	1	277.3	217.0	25.41	372	372	12647.5
5	4157.2	105.4	1	16.46	267.0	26.41	372	372	12777.4
6	4157.2	105.4	1	182.9	393.0				
7	4157.2	105.4	1	452.4	446.0	27.46	372	372	1571.6
8	4157.2	105.4	1	517.4	525.0	2.46	372	372	1543.1
9	41137.2	865.4	1	675.3	666.6	2.46	372	372	1517.1
10	41137.2	775.4	1	6641.2	6640.0	36.46	372	372	15414.4
11	41137.2	614.7	1	6496.5	6476.6	31.46	372	372	15427.0
12	41137.2	614.7	1	6123.9	6122.7	32.45	372	372	15433.0
13	41137.2	595.4	1	6774.9	6773.0	23.45	372	372	15452.0
14	41137.2	595.4	1	6317.2	6320.0				
15	41137.2	595.4	1	5965.0	6073.0				
CENT. C13%. CRYSTAL =									
16	41117.2	75.7	1	IC25C-E	IC25C-E				
17	41117.2	37.4	1	IC45.7	IC45.7				
18	41117.2	15.7	1	IC31.6	IC31.6				
19	41117.2	13.4	1	IC352.0	IC352.0				
20	41117.2	12.4	1	IC35.0	IC35.0				
21	41117.2	9.7	1	IC51.0	IC51.0				

BEST AVAILA  
BLE CAR

TABLE XIX. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS FOR  $\text{Er}^{3+}$  IN  $\text{YAlO}_3$ <sup>a</sup>

ER IN YALC3. SCALED $\Delta E_{\text{CP}}$ FROM PC DETERMINED BY AVERAGING DV AND FF IC-MED RESULTS									
INT.	8KM AND CENTRIFIDS.	Q = -G=0C,	-167.000 = 922	-R41.000 = 840	-470.000 = 942	325.000 = 842	-33.200 = 944	-544.000 = 944	-544.000 = 944
INT.	8KM AND CENTRIFIDS.	Q = -G=0C,	-61.000 = 862	-18t.000 = 862	575.000 = 864	-37.C30 = 864	-202.000 = 866	132.CCC = 866	132.CCC = 866
4115/2	265.0								
4113/2	5738.3								
4111/2	10348.0								
41 9/2	12965.3								
4F 9/2	15363.2								
45 3/2	18472.0								
2H11/2 2	13155.3								
4F 7/2	20562.3								
4F 5/2	22230.3								
4F 3/2	22561.3								
		FREE IDW	PCT PURE	ZNU	THEO. ENERGY	EXP. ENERGY			
		4-5	0-C			27 4F 9/2	93-3	1	15271.7
1 6115/2	97.9	1	69.5	0-C		28 4F 7/2	93-4	1	0-C
2 4115/2	162.6	1	173.0	1-C		29 4F 3/2	93-7	1	15371.3
3 4115/2	106.3	1	219.4	0-C		30 4F 9/2	93-7	1	0-C
4 4115/2	100.5	1	238.9	0-C		31 4F 3/2	93-9	1	15447.3
5 4115/2	103.3	1	153.7	0-C					
6 4115/2	106.2	1	662.9	0-C		32 4S 3/2	97-3	1	0-C
7 4115/2	106.6	1	542.9	0-C		33 4S 3/2	97-1	1	15421.1
8 4115/2	100.5	1	542.9	0-C					
9 4113/2	59.9	1	660.4	0-C		34 2H11/2 2	97-3	1	19112.7
10 4113/2	99.0	1	664.3	0-C		35 2H11/2 2	93-6	1	19133.0
11 4113/2	99.0	1	66P2.5	0-C		36 2H11/2 2	93-7	1	19183.1
12 4113/2	99.5	1	670.4	0-C		37 2H11/2 2	93-7	1	19205.6
13 4113/2	93.7	1	676.3	0-C		38 2H11/2 2	98-3	1	19242.7
14 4113/2	92.4	1	6912.6	0-C		39 2H11/2 2	94.5	1	19265.5
15 4113/2	93.7	1	6m8C-F	0-C					
16 4111/2	99.1	1	10281.4	0-C		40 4E 7/2	93-4	1	20544.5
17 4111/2	95.7	1	10350.7	0-C		41 4E 7/2	94-4	1	20501.4
18 4111/2	92.7	1	10431.0	0-C		42 4E 7/2	93-4	1	20594.5
19 4111/2	99.4	1	10449.3	0-C		43 4E 7/2	93-4	1	20594.5
20 4111/2	91.6	1	10375.6	0-C		44 4E 5/2	93-2	1	22221.5
21 4111/2	93.7	1	10418.5	0-C		45 4E 5/2	93-7	1	22217.7
						46 4E 5/2	93-4	1	22274.1
22 41 9/2	92.6	1	1239C.9	0-C		47 4F 3/2	92-2	1	22531.4
23 41 9/2	93.4	1	12462.7	0-C		48 4F 3/2	97-2	1	22626.2
24 41 9/2	99.3	1	12377.9	0-C					
25 41 9/2	92.4	1	12664.1	0-C					
26 41 9/2	93.1	1	12732.6	0-C					

<sup>a</sup> These  $B_{km}$  values were obtained by scaling the Ho parameters by the  $\rho_k$  value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological  $B_{km}$  values.

TABLE XX. ENERGY LEVELS AND PHENOMENOLOGICAL CRYSTAL FIELD PARAMETERS FOR Tm<sup>3+</sup> IN YAlO<sub>3</sub><sup>a</sup>

TP IN YALO <sub>3</sub> RUSSIAN DATA 9/17/75	FINAL BKM AND CENTRIFUGAL Q =	c-1t <sub>2</sub>	-783.364 = E <sub>43</sub>	-679.761 = E <sub>42</sub>	367.255 = E <sub>41</sub>	-56.332 = E <sub>44</sub>	-445.444 = E <sub>44</sub>
675.198 = E <sub>20</sub>	-75.502 = E <sub>21</sub>	-153.312 = E <sub>22</sub>	-153.312 = E <sub>23</sub>	620.311 = E <sub>24</sub>	59.227 = E <sub>24</sub>	-218.224 = E <sub>24</sub>	115.257 = E <sub>24</sub>
-752.332 = E <sub>25</sub>							
3W 6	342.0						
3F 4	586.6						
3H 5	8685.7						
3F 4	14546.4						
3F 2	15147.3						
1G 4	21343.5						
		FREE ICN PCF PDC	2DU THEO-E <sub>EXC-GV</sub>	EXP-ENERGY			
1	3H 6	73.3	2	-0.0	19.0	2	5531.0
2	3H 6	73.3	3	0.0	30.3	0	5531.0
3	3H 6	73.3	2	-0.0	31.3	0	5531.0
4	3H 5	73.3	0	-0.0	32.3	0	5531.0
5	3H 6	73.3	0	-0.0	33.3	0	5531.0
6	3H 6	ICCN	2	-0.0	34.3	0	5531.0
7	3H 5	100.1	2	-0.0	35.3	0	5531.0
8	3H 6	73.3	1	-0.0	36.3	0	5531.0
9	3H 6	73.3	0	-0.0	36.3	0	5531.0
10	3H 6	ICCN	2	-0.0	37.3	0	5531.0
11	3H 6	73.3	2	-0.0	38.3	0	5531.0
12	3H 5	102.0	3	-0.0	39.3	0	5531.0
13	3H 6	100.0	0	-0.0	40.3	0	5531.0
14	3F 4	33.7	2	5526.4	5631.0	0	15346.4
15	3F 4	33.7	2	5714.4	5713.0	0	15125.4
16	3F 5	33.7	0	5715.6	5722.0*	0	15137.2
17	3F 4	33.7	0	5823.2	5825.0	0	15197.4
18	3F 4	93.4	2	5830.4	5839.0*	0	15297.0
19	3F 4	93.5	0	5928.1	5912.0*	0	15287.0
20	3F 4	93.7	0	5492.0	-0.0	0	15287.0
21	3F 5	93.5	2	5779.2	-0.0	0	15287.0
22	3F 4	33.7	2	6135.4	-0.0	0	15287.0
23	3H 5	34.6	0	9371.1	-0.0	0	15287.0
24	3H 5	33.7	2	8257.4	8263.0	0	15287.0
25	3H 5	33.6	2	8133.4	8344.0	0	15287.0
26	3H 5	93.5	0	8377.0	8377.0	0	15287.0
27	3H 5	93.7	0	8449.3	8459.0	0	15287.0
28	3H 5	93.5	2	8511.3	8535.0	0	15287.0

<sup>a</sup>The least-rms deviation between the calculated and experimental energy levels is 6.16 cm<sup>-1</sup>.

TABLE XXI. CRYSTAL FIELD PARAMETERS,  $B_{km}$ , AND ENERGY LEVELS FOR  $Tm^{3+}$  IN  $YAlO_3$ <sup>a</sup>

		Tm IN $YAlO_3$ . SCALED FROM HQ DETERMINED BY AVERAGING DV AND EP HOPE'S RESULTS									
		INIT. BKP AND CENTERIDS.					-0.0.0				
		552.000 = R20 -169.000 = 8.27 -626.000 = R50 -462.000 = R42					-183.000 = R62 565.000 = R64 -38.000 = R64				
		-738.000 = R67 255.0 -198.000 = R63 130.000 = R66					-33.000 = R44 -198.000 = R66				
3H	6	255.0									
3F	4	5820.0									
3H	5	6435.0									
3H	4	12731.0									
3F	3	14529.3									
3F	2	15133.3									
1G	4	21325.3									
1D	2	27892.0									
		FREE ION PCF PURE 2PCF 3MED-ENERGY EXP-ENERGY									
1	3H	4	99.-3	0	-74.-2	0.-0	29 3H 5	99.-6	2	6473.8	1.-C
2	3H	6	99.-3	2	-68.-8	0.-0	30 3H 5	91.-5	0	6573.1	0.-C
3	3H	6	99.-9	2	31.-4	0.-0	31 3H 5	99.-6	0	5572.2	0.-C
4	3H	6	100.-0	0	62.-7	0.-0	32 3H 5	99.-7	2	617.1	0.-C
5	3H	6	99.-8	0	202.-6	0.-0	33 3H 5	99.-9	2	631.3	0.-C
6	3H	6	100.-0	2	242.-6	0.-0	34 3H 4	99.-5	0	12470.0	0.-C
7	3H	6	99.-9	2	287.-7	0.-0	35 3H 4	98.-8	2	12570.1	0.-C
8	3H	6	99.-9	0	123.-2	0.-0	36 3H 4	97.-6	2	12552.4	0.-C
9	3H	6	99.-6	0	192.-3	0.-0	37 3H 4	98.-8	0	12681.9	0.-C
10	3H	6	99.-9	2	392.-4	0.-0	38 3H 4	98.-8	2	12745.4	0.-C
11	3H	6	99.-3	2	460.-3	0.-0	39 3H 4	99.-2	2	12765.0	0.-C
12	3H	6	99.-9	0	494.-7	0.-0	40 3H 4	99.-4	0	12705.3	0.-C
13	3H	6	99.-3	0	505.-9	0.-0	41 3H 4	99.-6	0	12885.4	0.-C
14	3F	4	231.-7	0	5207.2	0.-0	42 3H 4	99.-3	0	12392.5	0.-C
15	3F	4	99.-4	2	5664.-9	0.-0	43 3F 3	98.-9	2	16470.9	0.-C
16	3F	4	93.-2	0	5630.1	0.-0	44 3F 3	94.-1	2	16434.7	0.-C
17	3F	4	94.-6	0	5777.-5	0.-0	45 3F 3	97.-3	0	14576.6	0.-C
18	3F	4	93.-4	2	5860.9	0.-0	46 3F 3	94.-3	2	14732.4	0.-C
19	3F	4	99.-5	0	5831.-6	0.-0	47 3F 3	94.-7	2	14560.3	0.-C
20	3F	4	93.-7	0	5925.-2	0.-0	48 3F 3	93.-7	0	14741.3	0.-C
21	3F	4	93.-7	2	5066.-9	0.-0	49 3F 3	97.-1	0	14514.6	0.-C
22	3F	4	93.-7	2	6602.-3	0.-0					
23	3H	5	211.-6	0	9197.3	0.-0					
24	3H	5	93.-0	2	6714.-7	0.-0					
25	3H	5	99.-0	2	6796.-6	0.-0					
26	3H	5	93.-5	0	6311.1	0.-0					
27	3H	5	79.-7	0	2445.-6	0.-0					
28	3H	5	94.-3	2	8460.-6	0.-0					

<sup>a</sup>See footnote at end of table.

TABLE XXI - CRYSTAL FIELD PARAMETERS,  $B_{Km}$ , AND ENERGY LEVELS  
FOR  $Tm^{3+}$  IN  $YAlO_3$  (CONT'D)

FREE ION	POL	POL	2MU	THEO. ENERGY	EXP. ENERGY
50 3F 2	34.7	0	15145.3	3.0	
51 4F 2	34.3	2	15136.5	3.0	
52 4F 2	37.8	0	15147.0	3.0	
53 3F 2	27.1	2	15164.5	3.0	
54 3F 2	36.6	0	15175.4	3.0	
55 1D 4	9.9	0	21621.8	0.0	
56 1G 4	24.7	2	21627.4	0.0	
57 1D 4	24.2	0	21622.6	0.0	
58 1D 4	16.5	0	21795.0	0.0	
59 1G 4	16.5	2	21404.3	0.0	
60 1G 4	10.4	0	21624.5	0.0	
61 1D 4	10.6	0	21477.5	0.0	
62 1G 4	10.6	2	21557.4	0.0	
63 1L 4	10.6	2	21521.5	2.0	
64 1G 2	49.3	0	27960.2	2.0	
65 1L 2	34.3	0	27424.5	2.0	
66 1L 2	16.6	2	27137.9	2.0	
67 1G 2	10.6	0	27163.5	2.0	
68 1F 2	10.6	2	27181.5	3.0	

<sup>a</sup> These  $B_{Km}$  values were obtained by scaling the Ho parameters by the  $\Omega_K$  value of table II. The Ho parameters were obtained by a linear interpolation of the Dy and Er phenomenological  $B_{Km}$  values.

TABLE XXII. AMPLITUDES, CRYSTAL FIELD COMPONENTS,  
 $A_{km}$  IN  $\text{cm}^{-1}$  Å-k, OF SPHERICAL DECOM-  
 POSITION OF  $\text{YAlO}_3$  LATTICE SUMS<sup>a</sup>

$k$	$m$	$K_{km}^{(1)}(q_0)$	$D$	$K_{km}^{(2)}(q_0)$	$-D$
1	0	-3811.7		16.77	
1	1	1703		0.99	
1	2	68.17		816.18	
1	3	-444.7		94.97	
1	4	-1836		1183	
1	5	-1025		1125	
1	6	-336.2		3230	
1	7	-321.3		627.0	
1	8	-1976		3918	
1	9	1996		4194.6	
1	10	-619.1		1231	
1	11	1452		826.2	
1	12	-812.3		1953	
1	13	-329.8		771.6	
1	14	53.93		128.1	
1	15	-272.7		932.4	
1	16	-1321		2673	
1	17	794.9		1815	
1	18	-738.4		1761	
1	19	32.35		60.47	
1	20	-231.1		564.4	
1	21	110.3		226.5	
1	22	435.9		1066	
1	23	121.9		243.6	
1	24	-282.9		719.6	
1	25	15.18		30.56	
1	26	-160.1		409.7	
1	27	-72.75		146.5	
1	28	-26.31		58.64	
1	29	13.59		27.87	
1	30	15.48		30.00	
1	31	-27.56		55.96	
1	32	-21.40		42.37	

The next morning I went to the station to get my train to the south. The station was at the end of the line, and there were no other stations between it and the coast.

The oxygen partial pressure dependence of the lattice constants taken at 400°C and 500°C respectively. The lattice constants of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> (JCPDS 33-066) and  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> (JCPDS 33-067) were used as reference. The atomic coordination number is 12.

Atom	$\gamma^{+}$	$\text{Al}^{+}$	O <sub>1</sub>	O <sub>11</sub>
Position	4a	4b	4c	8d
x	0.0526(2)	0	0.475(2)	0.293(2)
y	0.025	0	0.025	0.044(2)
z	0.9896(2)	0.050	0.086(2)	0.703(2)

TABLE XXXIII. AMPLITUDES, CRYSTAL FIELD COMPONENTS,  
 $A_{km}$ , IN  $\text{cm}^{-1} \text{\AA}^{-k}$ , OF SPHERICAL DECOM-  
 POSITION OF  $\text{YAlO}_3$  LATTICE SUMS FOR  
 EVEN VALUES OF  $k^2$

k	m	$A_{km} (\alpha_0 = -1)$		$A_{km} (\alpha_0 = +1, 3)$	
		Real	Imaginary	Real	Imaginary
2	0	2365.1	0	3482	0
2	1	0	-384.5	0	-466.2
2	2	610.3	0	615.4	0
4	0	-3749	0	-3321	0
4	1	0	1401	0	2108
4	2	698.2	0	1007	0
4	3	0	860.0	0	1274
4	4	-779.5	0	167.3	0
6	0	-285.6	0	-502.2	0
6	1	0	36.68	0	62.49
6	2	-67.11	0	-101.0	0
6	3	0	96.78	0	146.2
6	4	139.6	0	125.9	0
6	5	0	-92.15	0	-77.24
6	6	137.8	0	204.2	0

<sup>a</sup>The coordinate system has been rotated so that the real part of  $A_{km}$  is for  $m < 0$ . The lattice constants and atomic positions are given in Table XXII.

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